Methyl 3-hydroxybenzoate 19438-10-9 | DTXSID50173071

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Model Performance

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N	Model	Data	

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 95.8 °C

Global applicability domain: Inside

Local applicability domain index: 8.86e-01

Confidence level: 6.20e-01

Nearest Neighbors from the Training Set

Image not found

Methyl 3-hydroxybenzoate

Measured: 73.0 Predicted: 95.8

Image not found

Methylparaben
Measured: 131
Predicted: 98.7

Image not found

Ethylparaben
Measured: 117
Predicted: 101

Image not found

Ethyl 3-hydroxybenzoate

Measured: 74.0 Predicted: 93.5

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Propylparaben
Measured: 97.0
Predicted: 88.7